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# SHOCK TUBE MEASUREMENTS OF IGNITION PROCESSES IN DIESEL-RELATED FUELS

ARO contract - to begin June 1, 2001

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## SUMMARY/OVERVIEW

We are beginning a three-year program of basic research concerned with chemical kinetics of diesel and diesel fuel surrogates. The work is intended to support efforts underway in other laboratories to develop improved diesel engine performance. The research will be carried out in the Stanford shock tube facilities and will focus on two areas: (1) measurement of shock tube ignition times and individual species concentration time-histories in gas-phase diesel surrogates, and (2) investigation of the reactive behavior of fuel spray droplets in shock-heated gases. Both high-pressure and low-pressure shock tubes will be used in the gas-phase investigations, and a new facility will be assembled (from an existing shock tube) for fundamental studies of fuel sprays in shock-heated gases. Modern optical diagnostic techniques will be employed to build data sets for these reactive flows.

## TECHNICAL DISCUSSION

The research will involve (1) accurate measurements of ignition time and their use to create reliable correlations for a variety of diesel fuel surrogates, and blends of surrogates to simulate diesel, useful over wide ranges of temperature, pressure, fuel mole fraction, and stoichiometry, (2) measurements of individual species concentration time-histories behind shock waves to improve or validate detailed kinetic mechanisms and establish reduced mechanisms, (3) use of a new UV absorption kinetic spectrograph for the identification of transient fuel fragments, and (4) acquisition of data on fuel spray behavior that will aid development and validation of CFD models of spray break-up, evaporation and combustion.

Measurements of species concentration time-histories place stronger constraints on kinetic models than ignition times alone. Figure 1 shows a comparison of post-shock OH species time-histories for n-decane oxidation acquired using ring-dye laser absorption and modeled using the kinetic mechanism of Lindstedt and Maurice (1995). Though the modeled ignition times are within a factor of two of the experimental values, improvements in the model are clearly needed to bring the model results into agreement with the data.

The identification of elementary decomposition products of primary fuel components, and of transient intermediates in the combustion process, are also needed for development of correct kinetic mechanisms. Figure 2 shows two high temperature UV absorption spectra, that of 1,3-butadiene and cyclopentadiene, that were acquired using our recently acquired kinetic

spectrograph. This new diagnostic enables recording of broad absorption spectra (190-300 nm) at 10  $\mu$ s intervals, i.e. multiple spectra can be recorded in each shock tube kinetics experiment. The intermediates shown in Fig. 2 are expected to be present on the reaction pathway from diesel fuel decomposition and oxidation to aromatic and soot formation. By quantifying the absorption spectra of these and other intermediate fuel products, and recording time-resolved spectra using the kinetic spectrograph, we hope to identify the primary decomposition and oxidation pathways for diesel fuel surrogates and to build a data base for the time histories of these species in shock-heated mixtures.

The availability at Stanford of unique flow facilities (low and high-pressure shock tubes and a new shock tube spray combustion facility) and diagnostic capabilities (high-speed schlieren, PLIF, laser absorption, UV kinetic spectrograph, and other spectroscopic techniques) will enable acquisition of new and unique data on hydrocarbon fuel pyrolysis and oxidation, and lead eventually to improved, detailed kinetic models of combustion in engines.

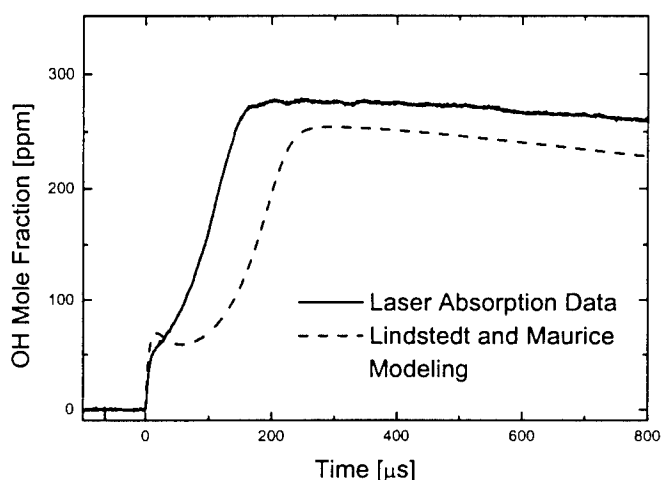


Fig. 1. n-Decane oxidation. A comparison of measured and calculated OH time-history in shock heated n-decane/oxygen/argon. Reflected shock conditions: 300 ppm n-decane,  $\phi = 1.0$ ,  $T = 1661$  K,  $P = 2.08$  atm

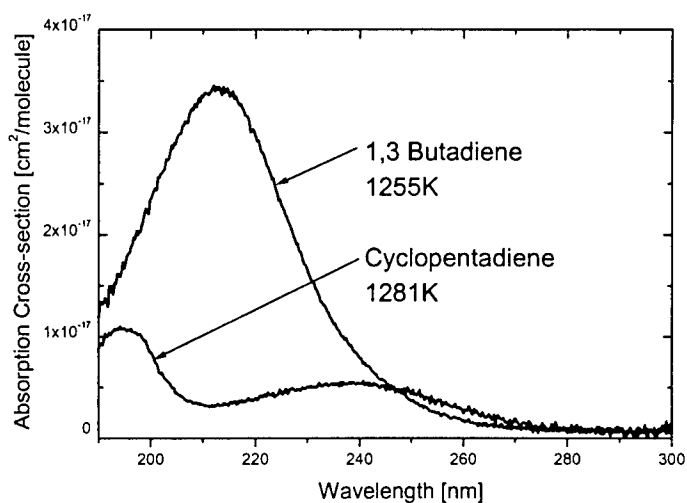


Fig. 2. UV absorption spectra of two dienes acquired behind reflected shock waves using the kinetic spectrograph. These and other high temperature spectra will be used to identify stable and transient decomposition products of diesel and diesel fuel surrogates